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* * * * * Welcome to STN International * * * * *

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NEWS 2 NOV 21 CAS patent coverage to include exemplified prophetic
substances identified in English-, French-, German-,
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NEWS 3 NOV 26 MARPAT enhanced with FSORT command
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NEWS 5 NOV 26 Two new SET commands increase convenience of STN
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NEWS 7 DEC 12 GBFULL now offers single source for full-text
coverage of complete UK patent families
NEWS 8 DEC 17 Fifty-one pharmaceutical ingredients added to PS
NEWS 9 JAN 06 The retention policy for unread STNmail messages
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NEWS 10 JAN 07 WPIDS, WPINDEX, and WPIX enhanced Japanese Patent
Classification Data
NEWS 11 FEB 02 Simultaneous left and right truncation (SLART) added
for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS 12 FEB 02 GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS 13 FEB 06 Patent sequence location (PSL) data added to USGENE
NEWS 14 FEB 10 COMPENDEX reloaded and enhanced
NEWS 15 FEB 11 WTEXTILES reloaded and enhanced

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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NEWS IPC8 For general information regarding STN implementation of IPC 8

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 12:04:13 ON 17 FEB 2009

=> FIL CASREACT

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.22

0.22

FILE 'CASREACT' ENTERED AT 12:04:26 ON 17 FEB 2009

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FILE CONTENT:1840 - 8 Feb 2009 VOL 150 ISS 7

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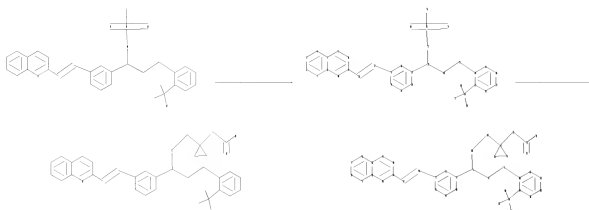
```
*****
*
*   CASREACT now has more than 16.5 million reactions
*
*****
```

CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10-576,971.str



```

chain nodes :
11 12 19 20 21 28 29 30 31 32 33 34 35 36 47 48 55 56 57 64 65
66 67 68 69 71 72 73 74
ring nodes :
1 2 3 4 5 6 7 8 9 10 13 14 15 16 17 18 22 23 24 25 26 27 37
38 39 40 41 42 43 44 45 46 49 50 51 52 53 54 58 59 60 61 62 63
70 75 76
chain bonds :
9-11 11-12 12-15 17-19 19-20 19-32 20-21 21-24 23-28 28-29 28-30 28-31
32-33 33-34 33-35 33-36 45-47 47-48 48-51 53-55 55-56 55-68 56-57 57-60
59-64 64-65 64-66 64-67 68-69 69-70 70-71 71-72 72-73 72-74
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 13-14 13-18 14-15 15-16
16-17 17-18 22-23 22-27 23-24 24-25 25-26 26-27 37-38 37-42 38-39 39-40
40-41 41-42 41-43 42-46 43-44 44-45 45-46 49-50 49-54 50-51 51-52 52-53
53-54 58-59 58-63 59-60 60-61 61-62 62-63 70-75 70-76 75-76
exact/norm bonds :
19-32 28-29 32-33 33-34 33-35 33-36 55-68 64-65 68-69 72-73 72-74
exact bonds :
9-11 11-12 12-15 17-19 19-20 20-21 21-24 23-28 28-30 28-31 45-47 47-48
48-51 53-55 55-56 56-57 57-60 59-64 64-66 64-67 69-70 70-71 70-75 70-76
71-72 75-76
normalized bonds :

```

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 13-14 13-18 14-15 15-16
16-17 17-18 22-23 22-27 23-24 24-25 25-26 26-27 37-38 37-42 38-39 39-40
40-41 41-42 41-43 42-46 43-44 44-45 45-46 49-50 49-54 50-51 51-52 52-53
53-54 58-59 58-63 59-60 60-61 61-62 62-63

isolated ring systems :

containing 1 : 13 : 22 : 37 : 49 : 58 : 70 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS
37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom
46:Atom 47:CLASS 48:CLASS 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom
55:CLASS 56:CLASS 57:CLASS 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom
64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:Atom 71:CLASS
72:CLASS 73:CLASS 74:CLASS 75:Atom 76:Atom

fragments assigned reactant/reagent role:

containing 1

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 12:05:24 FILE 'CASREACT'

SCREENING COMPLETE - 2 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 2 VERIFIED 2 HIT RXNS 1 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 2 TO 124

PROJECTED ANSWERS: 1 TO 79

L2 1 SEA SSS SAM L1 (2 REACTIONS)

=> s l1 sss full

FILE SEARCH INITIATED 12:05:52 FILE 'CASREACT'

SCREENING COMPLETE - 77 REACTIONS TO VERIFY FROM 21 DOCUMENTS

100.0% DONE 77 VERIFIED 57 HIT RXNS 16 DOCS

SEARCH TIME: 00.00.01

L3 16 SEA SSS FUL L1 (57 REACTIONS)

02/18/2009

10-576,971.trn

=> d occ 1-

YOU HAVE REQUESTED DATA FROM 16 ANSWERS - CONTINUE? Y/(N):y

02/18/2009

10-576,971.trn

L3 ANSWER 1 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
NUMBER OF HIT REACTIONS 2
NUMBER OF REACTIONS IN PATH 2
NUMBER OF REACTIONS IN STATE 2
FIELD COUNT
FK(1) 2
FK(13) 2

L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
NUMBER OF HIT REACTIONS 6
NUMBER OF REACTIONS IN PATH 2
NUMBER OF REACTIONS IN STATE 2
FIELD COUNT
FK(1) 2
FK(4) 2
FK(5) 2
FK(6) 2
FK(9) 2
FK(10) 2

L3 ANSWER 3 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
NUMBER OF HIT REACTIONS 1
NUMBER OF REACTIONS IN PATH 1
NUMBER OF REACTIONS IN STATE 1
FIELD COUNT
FK(1) 2

L3 ANSWER 4 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
NUMBER OF HIT REACTIONS 1
NUMBER OF REACTIONS IN PATH 1
NUMBER OF REACTIONS IN STATE 1
FIELD COUNT
FK(1) 2

02/18/2009

10-576,971.trn

L3 ANSWER 5 OF 16 CASREACT	COPYRIGHT 2009 ACS on STM
NUMBER OF HIT REACTIONS	5
NUMBER OF REACTIONS IN PATH	3
NUMBER OF REACTIONS IN STATE	5
FIELD	COUNT
KX(1)	2
KX(3)	2
KX(6)	2
KX(9)	2
KX(12)	2

L3 ANSWER 6 OF 16 CASREACT	COPYRIGHT 2009 ACS on STM
NUMBER OF HIT REACTIONS	4
NUMBER OF REACTIONS IN PATH	1
NUMBER OF REACTIONS IN STATE	1
FIELD	COUNT
KX(1)	2
KX(7)	2
KX(9)	2
KX(10)	2

L3 ANSWER 7 OF 16 CASREACT	COPYRIGHT 2009 ACS on STM
NUMBER OF HIT REACTIONS	2
NUMBER OF REACTIONS IN PATH	2
NUMBER OF REACTIONS IN STATE	3
FIELD	COUNT
KX(1)	2
KX(3)	2
KX(4)	2

L3 ANSWER 8 OF 16 CASREACT	COPYRIGHT 2009 ACS on STM
NUMBER OF HIT REACTIONS	2
NUMBER OF REACTIONS IN PATH	1
NUMBER OF REACTIONS IN STATE	2
FIELD	COUNT
KX(1)	2
KX(2)	2

02/18/2009

10-576,971.trn

L3 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
 NUMBER OF HIT REACTIONS 4
 NUMBER OF REACTIONS IN PATH 1
 NUMBER OF REACTIONS IN SPATH 2
 FIELD COUNT
 FK(1) 2
 FK(4) 2
 FK(16) 2
 FK(13) 2

L3 ANSWER 10 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
 NUMBER OF HIT REACTIONS 4
 NUMBER OF REACTIONS IN PATH 4
 NUMBER OF REACTIONS IN SPATH 4
 FIELD COUNT
 FK(1) 2
 FK(2) 2
 FK(3) 2
 FK(4) 2

L3 ANSWER 11 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
 NUMBER OF HIT REACTIONS 2
 NUMBER OF REACTIONS IN PATH 2
 NUMBER OF REACTIONS IN SPATH 2
 FIELD COUNT
 FK(2) 2
 FK(13) 2

L3 ANSWER 12 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
 NUMBER OF HIT REACTIONS 4
 NUMBER OF REACTIONS IN PATH 2
 NUMBER OF REACTIONS IN SPATH 2
 FIELD COUNT
 FK(13) 2
 FK(15) 2
 FK(22) 2
 FK(24) 2
 FK(25) 2
 FK(30) 2

02/18/2009

10-576,971.trn

L3 ANSWER 13 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
NUMBER OF HIT REACTIONS 2
NUMBER OF REACTIONS IN PATH 1
NUMBER OF REACTIONS IN SPATH 2
FIELD COUNT
KX(12) 2
KX(15) 2

L3 ANSWER 14 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
NUMBER OF HIT REACTIONS 2
NUMBER OF REACTIONS IN PATH 1
NUMBER OF REACTIONS IN SPATH 2
FIELD COUNT
KX(12) 2
KX(13) 2

L3 ANSWER 15 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
NUMBER OF HIT REACTIONS 1
NUMBER OF REACTIONS IN PATH 1
NUMBER OF REACTIONS IN SPATH 1
FIELD COUNT
KX(8) 2

L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
NUMBER OF HIT REACTIONS 12
NUMBER OF REACTIONS IN PATH 1
NUMBER OF REACTIONS IN SPATH 1
FIELD COUNT
KX(4) 2
KX(10) 2
KX(17) 2
KX(18) 2
KX(20) 2
KX(21) 2
KX(23) 2
KX(24) 2
KX(25) 2
KX(26) 2
KX(27) 2
KX(28) 2

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=> d ibib abs hit

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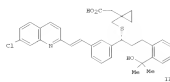
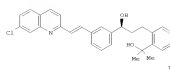
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L1 ANMER 1 OF 16 CASREACT COPYRIGHT 2009 ACS on STM
ACCESSION NUMBER: 149156436 CASREACT
TITLE: Process for the purification of optically pure
2:12-(3-(5)-(3-(7-thioloo-2-quinolinsyl)ethyl)phenyl)-3-
hydroxypropylphenyl-2-propanol.
INVENTOR(S):
Solomon, Ady; Gafni, Yael; Neuman, Alex; Perelman,
Dibara; Levin, Zeev; Nolsan, Michal; Altier, Ofir
PATENT ASSIGNER(S):
SOURCE:
Chemical Ltd., Israel
PCT int. Appl., 19pp.
CISN2: P1422
FAMILY ACC. NUM. COUNT: Patent
English
1

```

[illegible]

13 ANSWER 1 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



AS A process for trifluorinating an optically impure
2-[2-(11E)-3-[7-(chloro-2-quinolinyl)-
ethyl]-phenyl]-3-(hydroxypropyl)phenyl]-2-propanol (I) is disclosed.
The purified compound typically has an enantiomeric excess higher than
99%,
and can be used to prepare montelukast (II) and salts thereof.

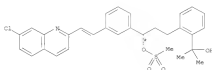
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT:

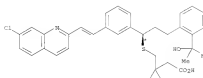
$$\text{Fig. (2) OP: } 5 \quad \dots G + C + H \implies Y$$


2

1.3 ANSWER 1 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



C



2: CM 2
 YIELD 796

8K(2) 8C7 G 162515-69-6

```

STAGE(1)
SOL 109-99-9 THF
CON SITESTAGE(1) 10 minutes, room temperature
SITESTAGE(2) room temperature -5 -15 deg

```

```
STAGE(2)
RGT J 109-72-8 BuLi
EOL 110-54-3 Benzene
CON SUBSTAGE(2) 75 minutes, -5 deg C
SUBSTAGE(2) 30 minutes, -5 deg C
```

STAGE(3)
RCT C 807638-71-7

1.3 ANSWER 1 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

```

SOL 109-99-9 THF
CON SUBSTAGE (1) -5 deg C
    SUBSTAGE (2) -5 deg C

```

```
STAGE(4)
RGT K 7647-14-5 NaCl
SOL 141-78-6 AcOEt, 7732-18-5 Water
CON SURSTAGE(1) 75 minutes, -5 deg C
SURSTAGE(2) 8.5 hours, -5 deg C -> room temperature
```

STAGE(5)
SOL 141-78-6 AcOEt
CON 30 minutes, 20 deg C

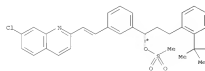
STAGE (6)
RCT R 101-83-7
CON 1 hour, 20 deg C

```
STAGE(7)
    BCL 110-54-3 Hexane
    CON SUBSTAGE(1) 2 hours,
```

PRO I 577953-88-9
NTE fourth stage quench; sixth stage seeding after clear soil

$$\text{KX}(3) \text{ OF } 5 \quad \dots G + C \implies P$$


6



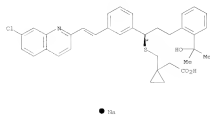
C

(3) ~

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10-576,971.trn

L3 ANSWER 1 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



P

XX(3) RCT G 162555-68-6

STAGE(1)
 SOL 129-99-9 THF
 CRI SUBSTAGE(1) 20 minutes, room temperature
 SUBSTAGE(2) room temperature -> -35 deg C

STAGE(2)
 RCT Z 109-72-8 BuLi
 SOL 112-54-3 Hexane
 CRI SUBSTAGE(1) 75 minutes, -5 deg C
 SUBSTAGE(2) 30 minutes, -5 deg C

STAGE(3)
 RCT G 807638-71-7
 SOL 129-99-9 THF
 CRI SUBSTAGE(1) -5 deg C
 SUBSTAGE(2) -5 deg C

STAGE(4)
 RCT X 7647-24-5 NaCl
 SOL 141-78-6 AcOEt, 7732-18-5 Water
 CRI SUBSTAGE(1) 75 minutes, -5 deg C
 SUBSTAGE(2) 8.5 hours, -5 deg C -> room temperature

STAGE(5)
 SOL 141-78-6 AcOEt
 CRI SUBSTAGE(1) 30 minutes, 20 deg C

STAGE(6)
 RCT R 101-83-7 Diisopropylamine
 CRI 2 hours, 20 deg C

L3 ANSWER 1 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

STAGE(7)
 SOL 110-54-3 Hexane
 CRI SUBSTAGE(1) 2 hours, 20 deg C
 SUBSTAGE(2) overnight, 20 deg C

STAGE(8)
 SOL 105-88-3 PIMe, 7732-18-5 Water
 CRI room temperature

STAGE(9)
 RCT Q 64-19-7 AcOH
 SOL 7732-18-5 Water
 CRI 10 minutes, 20 - 25 deg C

STAGE(10)
 SOL 7732-18-5 Water
 CRI 10 minutes, 20 - 25 deg C

STAGE(11)
 RCT R 1330-73-2 NaOH
 SOL 7732-18-5 Water, 64-17-5 EtOH
 CRI SUBSTAGE(1) 10 minutes, 20 - 25 deg C
 SUBSTAGE(2) 10 minutes, 20 - 25 deg C

STAGE(12)
 SOL 75-05-8 NaCl
 CRI SUBSTAGE(1) 20 minutes, 40 deg C
 SUBSTAGE(2) 1.5 hours, 40 deg C

STAGE(13)
 SOL 75-05-8 NaCl
 CRI SUBSTAGE(1) 20 minutes, 40 deg C
 SUBSTAGE(2) 1 hour, 40 deg C

STAGE(14)
 SOL 75-05-8 NaCl
 CRI SUBSTAGE(1) 20 minutes, 40 deg C
 SUBSTAGE(2) 1 hour, 40 deg C

PRO P 151767-02-1
 RTE Fourth stage quench; sixth stage seeding after clear soln.

02/18/2009

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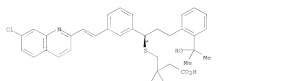
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YOU HAVE REQUESTED DATA FROM 16 ANSWERS - CONTINUE? Y/(N):y

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10-576,971.trn

L3 ANSWER 1 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



● Na

P

EX(7) RCT G 162555-68-6

STAGE(1)
SOL 129-99-9 THF
CON SUBSTAGE(1) 10 minutes, room temperature
SUBSTAGE(2) room temperature -> -35 deg C

STAGE(2)
RPT 7 109-72-8 BuLi
SOL 119-54-3 Benzene
CON SUBSTAGE(1) 15 minutes, -5 deg C
SUBSTAGE(2) 30 minutes, -5 deg C

STAGE(3)
RCT 6 807638-71-7
SOL 109-99-9 THF
CON SUBSTAGE(1) -5 deg C
SUBSTAGE(2) -5 deg C

STAGE(4)
RPT 8 7647-24-5 NaCl
SOL 141-78-6 AcOH, 7732-18-5 Water
CON SUBSTAGE(1) 75 minutes, -5 deg C
SUBSTAGE(2) 8.5 hours, -5 deg C -> room temperature

STAGE(5)
SOL 141-78-6 AcOH
CON 30 minutes, 20 deg C

STAGE(6)
RPT 8 101-83-7 Bioprotection
CON 2 hours, 20 deg C

L3 ANSWER 1 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

STAGE(7)
SOL 110-54-3 Benzene
CON SUBSTAGE(1) 2 hours, 20 deg C
SUBSTAGE(2) overnight, 20 deg C

STAGE(8)
SOL 105-88-3 PMS, 7732-18-5 Water
CON room temperature

STAGE(9)
RPT 9 44-19-7 AcOH
SOL 7732-18-5 Water
CON 10 minutes, 20 - 25 deg C

STAGE(10)
SOL 7732-18-5 Water
CON 10 minutes, 30 - 25 deg C

STAGE(11)
RPT 8 1330-73-2 NaOH
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) 10 minutes, 20 - 25 deg C
SUBSTAGE(2) 10 minutes, 20 - 25 deg C

STAGE(12)
SOL 75-05-8 NaOH
CON SUBSTAGE(1) 20 minutes, 40 deg C
SUBSTAGE(2) 1.5 hours, 40 deg C

STAGE(13)
SOL 75-05-8 NaOH
CON SUBSTAGE(1) 20 minutes, 40 deg C
SUBSTAGE(2) 1 hour, 40 deg C

STAGE(14)
SOL 75-05-8 NaOH
CON SUBSTAGE(1) 20 minutes, 40 deg C
SUBSTAGE(2) 1 hour, 40 deg C
RTE P 151767-02-3
NOTE Fourth stage quench; sixth stage seeding after clear soln.

L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:

TITLE

INVENTOR(S):

PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

FAMILY ACC. NUM. COUNTRY:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008136693	A2	20081113	WO 2008-PL33	20080430
WO 2008136693	A3	20091223		
W	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BE, CA, CB, CC, CD, CH, CI, CL, CN, CO, CR, CU, CY, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GM, GR, GT, HK, HU, IL, IN, JP, KE, KG, KP, KR, KZ, LA, LC, LI, LU, LV, LY, MA, MG, MK, MN, MU, MW, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PK, PL, PT, RU, RW, SA, SD, SE, SG, SI, SK, SL, SM, SN, SV, SY, TD, TH, TJ, TK, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VE, VN, YU, ZA, ZM, ZW			
BM	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BE, CA, CB, CC, CD, CH, CI, CL, CN, CO, CR, CU, CY, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GM, GR, GT, HK, HU, IL, IN, JP, KE, KG, KP, KR, KZ, LA, LC, LI, LU, LV, LY, MA, MG, MK, MN, MU, MW, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PK, PL, PT, RU, RW, SA, SD, SE, SG, SI, SK, SL, SM, SN, SV, SY, TD, TH, TJ, TK, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VE, VN, YU, ZA, ZM, ZW			
BM	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BE, CA, CB, CC, CD, CH, CI, CL, CN, CO, CR, CU, CY, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GM, GR, GT, HK, HU, IL, IN, JP, KE, KG, KP, KR, KZ, LA, LC, LI, LU, LV, LY, MA, MG, MK, MN, MU, MW, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PK, PL, PT, RU, RW, SA, SD, SE, SG, SI, SK, SL, SM, SN, SV, SY, TD, TH, TJ, TK, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VE, VN, YU, ZA, ZM, ZW			

PRIORITY APPL. INFO:

As Amorphous Montelukast sodium was prepared by (1) reaction of 2-[12-[18]-(9-[12-(7-chloro-2-quinolylmethyl)phenyl]-3-[12-(1-hydroxypropyl)phenyl]-2-propanol) with NaOH(1) in the presence of a tertiary amine, (2) filtration of precipitated tertiary amine salt and reaction of the crude methanesulfonate ester with [1-mercaptoethyl]cyclopropylacetic acid sodium salt, (3) isolation of crystalline 1-[[[18]-(12-[12-(7-chloro-2-quinolylmethyl)phenyl]-3-[12-(1-hydroxy-2-methylphenyl)propyl]sulfinyl)methyl]cyclopropanesulfonate and tert-butylamine salt, (4) purification of this salt until the product has high pharmaceutical purity, and (5) conversion of the purified salt to the title compound

EX(7) OF 10 --O + B + I ==> J

L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

ACCESSION NUMBER:

TITLE

INVENTOR(S):

PATENT ASSIGNEE(S):

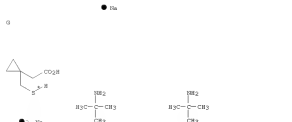
SOURCE:

DOCUMENT TYPE:

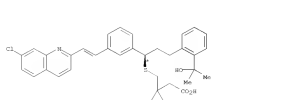
LANGUAGE:

FAMILY ACC. NUM. COUNTRY:

PATENT INFORMATION:



J: CM 1



J: CM 2

EX(7) RCT G 1079902-34-3, B 884842-91-5

STAGE(1)
CON SUBSTAGE(2) 12 hours, 30 - 15 deg C

02/18/2009

10-576,971.trn

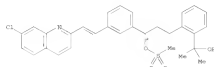
L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

STAGE(2)

RCT 1 75-64-9
 CON SUBSTAGE(1) 30 minutes
 PRO J 851755-58-3
 RTE workup

RX(4) OF 10

1. G + B ==> K



● Ha

G

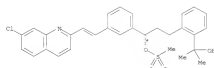


● Ha

(4) →

B

L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



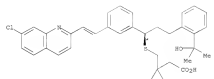
● Ha

G

2
 STERS →



J: CH 1

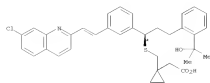


J: CH 2

RX(1) RCT A 162515-68-6
 RCT C 865-68-9 NaOtu-t
 PRO B 884842-91-5
 SOL 6H-12-3 THF
 CON SUBSTAGE(1) 20 +/- 5 deg C
 CON SUBSTAGE(2) 1 hour, >15 deg C

RX(3) RCT G 1079902-34-3, B 884842-91-5

L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



● Ha

K

RX(4) RCT G 1079902-34-3, B 884842-91-5

STAGE(1)

CON SUBSTAGE(2) 12 hours, 10 - 15 deg C

STAGE(2)

RCT 1 75-64-9 t-BuOH

CON SUBSTAGE(2) 30 minutes

STAGE(3)

RCT 1 64-19-7 AcOH

SOL 7732-18-5 MeOH

CON room temperature

STAGE(4)

RCT H 1310-73-2 NaOH

SOL 67-56-1 MeOH

CON room temperature

PRO K 151767-02-1

RX(1) OF 10 COMPOSED OF RX(1), RX(3)

RX(5) A + G + I ==> J



A

L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

STAGE(1)

CON SUBSTAGE(2) 12 hours, 10 - 15 deg C

STAGE(2)

RCT 1 75-64-9

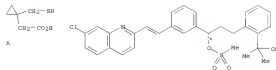
CON SUBSTAGE(2) 30 minutes

PRO J 851755-58-3

RTE workup

RX(6) OF 10 COMPOSED OF RX(1), RX(4)

RX(6) A + G ==> F

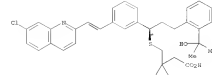


A

● Ha

G

2
 STERS →



K

RX(1) RCT A 162515-68-6
 RCT C 865-68-9 NaOtu-t
 PRO B 884842-91-5

L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

SOL 68-12-2 DMF
SUBSTAGE(1) 20/-5 deg C
CON SUBSTAGE(1) 1 hour, >15 deg C

RK(14) NCT G 1079902-34-3, B 884842-91-5

STAGE(1)
CON SUBSTAGE(2) 12 hours, 20 - 15 deg C

STAGE(2)
NCT 1 75-64-9 1-hydroxy
CON SUBSTAGE(2) 30 minutes

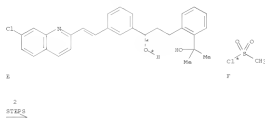
STAGE(3)
NCT 1 64-19-7 AcOH
SOL 7732-18-5 Mezep
CON room temperature

STAGE(4)
NCT B 1310-73-2 NaOH
SOL 67-56-1 MeOH
CON room temperature

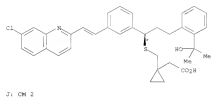
PRO K 151767-02-1

RK(9) OF 10 COMPOSED OF REACTION SEQUENCE RK(1), RK(3)
AND REACTION SEQUENCE RK(1), RK(3)

...E + F ==> G...
...A + G + 1 ==> J



L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



RK(12) NCT E 287930-77-2, F 124-63-0
NCT B 121-44-8 Et3N
PRO G 1079902-34-3
SOL 68-12-2 DMF
CON SUBSTAGE(1) room temperature -> -15 deg C
SUBSTAGE(2) -20 - -15 deg C
SUBSTAGE(3) 40 minutes

RK(11) NCT A 16255-68-6
NCT C 865-48-5 NaOH=t
PRO B 884842-91-5
SOL 68-12-2 DMF
CON SUBSTAGE(1) 20/-5 deg C
SUBSTAGE(2) 1 hour, >15 deg C

RK(13) NCT G 1079902-34-3, B 884842-91-5

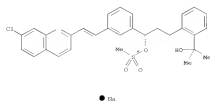
STAGE(1)
CON SUBSTAGE(2) 12 hours, 20 - 15 deg C

STAGE(2)
NCT 1 75-64-9
CON SUBSTAGE(2) 30 minutes

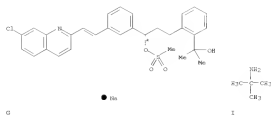
PRO J 851755-58-3
NTE workup

RK(16) OF 10 COMPOSED OF REACTION SEQUENCE RK(2), RK(4)
AND REACTION SEQUENCE RK(1), RK(4)

L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

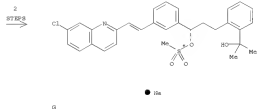
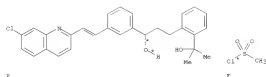


START NEXT REACTION SEQUENCE

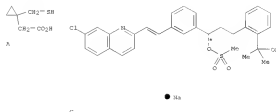


L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

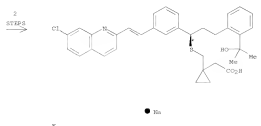
...E + F ==> G...
...A + G ==> K



START NEXT REACTION SEQUENCE



L3 ANSWER 2 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



F

KX(2) RCT E 287930-77-2, F 324-63-Q
 RUT B 123-44-9 E339
 PRO G 1279902-34-3
 SOL 68-12-2 DMF
 COR SUBSTANCE(1) room temperature -> -15 deg C
 SUBSTANCE(2) -20 - -15 deg C
 SUBSTANCE(3) 40 minutes

KX(1) RCT A 162555-68-6
 RUT C 985-48-5 NaOMe-t
 PRO B 884842-91-5
 SOL 68-12-3 DMF
 COR SUBSTANCE(1) 20/-5 deg C
 SUBSTANCE(3) 1 hour, >15 deg C

KX(4) RCT G 1079902-34-3, B 884842-91-5
 STAGE(1)
 COR SUBSTANCE(2) 12 hours, 10 - 15 deg C

STAGE(2)
 RUT J 75-44-9 t-BuNEt
 COR SUBSTANCE(2) 30 minutes

STAGE(3)
 RUT L 64-39-7 AcOH
 SOL 7152-18-5 Water
 COR room temperature

STAGE(4)
 RUT M 1310-73-2 NaOH
 SOL 67-56-1 MeOH

L3 ANSWER 3 OF 16 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:

TITLE:

INVENTOR(S):

PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008036335	A1	20080717	WO 2008-022	20080610
US	XX	XX	XX	XX
CA	XX	XX	XX	XX
JP	XX	XX	XX	XX
RU	XX	XX	XX	XX
BR	XX	XX	XX	XX
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FM	XX	XX	XX	XX
FO	XX	XX	XX	XX
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HG	XX	XX	XX	XX
HH	XX	XX	XX	XX
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IV	XX	XX	XX	XX
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LS	XX	XX	XX	XX
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LU	XX	XX	XX	XX
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LY	XX	XX	XX	XX
MA	XX	XX	XX	XX
MC	XX	XX	XX	XX
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MI	XX	XX	XX	XX
MJ	XX	XX	XX	XX
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NY	XX	XX	XX	XX
NZ	XX	XX	XX	XX
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OC	XX	XX	XX	XX
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OG	XX	XX	XX	XX
OH	XX	XX	XX	XX
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OJ	XX	XX	XX	XX
OK	XX	XX	XX	XX
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OO	XX	XX	XX	XX
OP	XX	XX	XX	XX
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PR	XX	XX	XX	XX
PS	XX	XX	XX	XX
PT	XX	XX	XX	XX
PV</				

L3 ANSWER 4 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)
 ACCESSION NUMBER: 149133029 CASREACT
 TITLE: Improved process for preparation of
 (R)-1-[3-[[1-[[1-[2-[[7-chloro-2-
 quinolinyloxy]phenyl]-2-(1-hydroxy-1-
 methyl-ethyl)phenyl]thio]methyl]cyclopropyl]acetic acid
 acid
 dicyclohexylamine salt (montelukast dicyclohexylamine
 salt)
 INVENTOR(S): Ravi, Ruchi; Ruddy; Balilichand, Satyanarayana;
 Srinivas, Venka Venkata Naga Chandra Sekhar
 PATENT ASSIGNOR(S): Dr. Ruddy's Laboratories Limited, India
 SOURCE: Indian Pat. Appl., 10pp.
 CODES: INAKO Patent
 DOCUMENT TYPE: English
 LANGUAGE: English
 FAMILY ACT. NUM. COUNT: 1
 PATENT INFORMATION:

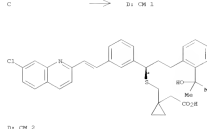
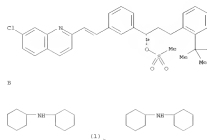
PATENT NO. KIND DATE APPLICATION NO. DATE
 IN 2006M00307 A 20070803 IN 2002-MA307 20020422
 PRIORITY APPL. INFO.: IN 2002-MA307 20020422
 AB The present invention provides the novel receptor, method for the
 preparation of
 of (R)-1-[3-[[1-[[1-[2-[[7-chloro-2-quinolinyloxy]phenyl]-2-(1-hydroxy-1-
 methyl-ethyl)phenyl]thio]methyl]cyclopropyl]acetic acid
 dicyclohexylamine salt (montelukast dicyclohexylamine salt). The novel
 receptor, method involves the purification of crude montelukast
 dicyclohexylamine salt in a mixture of nitriles and alcohols such as
 acetonitrile and methanol or 2-propanol.

EX(1) OF 1 A + B + C ==> D



A

L3 ANSWER 4 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



EX(1) RCT A 161515-68-6

STAGE(1)
 RCT 8 109-72-8 RSL
 SOL 109-99-9 THF
 CDM SUBSTAGE(1) room temperature -> -15 deg C
 SUBSTAGE(2) 1 hour, -10 deg C
 SUBSTAGE(3) 30 minutes, -10 deg C
 STAGE(2)
 RCT B 807638-71-7
 SOL 109-99-9 THF
 CDM SUBSTAGE(1) -10 deg C

L3 ANSWER 4 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)
 SUBSTAGE(2) 10 - 12 hours, -5 - 0 deg C

STAGE(3)
 RCT C 151-83-7
 SOL 141-78-6 AcOEt
 PRO D 577953-88-9

L3 ANSWER 5 OF 16 CASREACT COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 149111404 CASREACT
 TITLE: A process for the preparation of leukotriene receptor
 antagonist (montelukast sodium)
 INVENTOR(S): Ray, Gitan Komar; Ray, Sreenivasulu; Pathana,
 Sreenivasa Ravi Monnakshimundaram, Sivakumaran
 PATENT ASSIGNOR(S): Aureliochem Pharma Limited, India
 SOURCE: PCT Int. Appl., 27pp.
 CODES: PTA02
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACT. NUM. COUNT: 1
 PATENT INFORMATION:

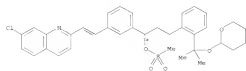
PATENT NO. KIND DATE APPLICATION NO. DATE
 WO 2006012113 A1 20060103 WO 2007-121970 20070425
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 W2 AT, BG, BR, CA, CH, CN, CO, CU, CY, CZ, DE, DK, EE, FI, FR, GB, GR, HU, IE, IS, IT, JP, KR, LV, LU, MA, MD, ME, MG, MK, MN, MU, MY, NL, NO, NZ, OM, OS, PA, PE, PG, PH, PL, PT, RU, SE, SI, SK, TH, TR, TT, TZ, UA, US, UZ, VC, VN, ZA, ZM, ZW
 W3 AU, BG, BR, CA, CH, CN, CO, CU, CY, CZ, DE, DK, EE, FI, FR, GB, GR, HU, IE, IS, IT, JP, KR, LV, LU, MA, MD, ME, MG, MK, MN, MU, MY, NL, NO, NZ, OM, OS, PA, PE, PG, PH, PL, PT, RU, SE, SI, SK, TH, TR, TT, TZ, UA, US, UZ, VC, VN, ZA, ZM, ZW
 IN 2006C01084 A 20061128 IN 2006-CH1084 20060626
 IN 2006C01085 A 20061128 IN 2006-CH1085 20060626
 PRIORITY APPL. INFO.: IN 2006-CH1084 20060626
 IN 2006-CH1085 20060626
 AB The invention relates to a process for the preparation of
 1-[[11R]-3-[[1-[[1R]-2-[[7-chloro-2-quinolinyloxy]phenyl]-2-(1-hydroxy-1-methyl-ethyl)phenyl]thio]methyl]cyclopropyl]acetic acid,
 monosodium salt, known as montelukast sodium.
 REFERENCE COUNT: 4 THESE ARE CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE EE
 FORMAT

EX(1) OF 14 ...A + B ==> C



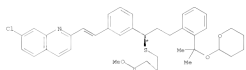
A

L3 ANSWER 5 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



B

(1) →



C

YIELD 73%

EX(1): RCT A 152922-73-5, B 162489-71-6
 RCT D 584-08-7 K2CO3
 PRO C 1000788-70-4
 SOL 75-03-8 MeCN
 SUBSTAGE(1) 27 - 30 deg C
 SUBSTAGE(2) 1 hour, -5 - 0 deg C
 SUBSTAGE(3) 0 deg C → 30 deg C
 SUBSTAGE(4) 36 hours, 27 - 30 deg C

EX(3) OF 14 ...R + A ==> K...

L3 ANSWER 5 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

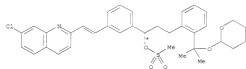
CON SUBSTAGE(1) 15 minutes, -5 - 0 deg C
 SUBSTAGE(2) 0 deg C → 20 deg C
 SUBSTAGE(3) 36 hours, 20 - 25 deg C

PRO K 855473-51-7

EX(6) OF 14 ...T + B ==> U...



T



B

(6) →

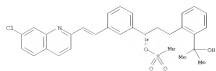


U

EX(6) RCT T 162555-68-6

STAGE(1)
 RCT V 1029-72-8 BuLi
 SOL 1029-89-9 THF
 CON SUBSTAGE(1) 25 - 30 deg C
 SUBSTAGE(2) 30 deg C → -15 deg C
 SUBSTAGE(3) 30 minutes, -5 deg C

L3 ANSWER 5 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

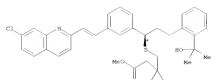


H



A

(3) →



K

YIELD 99%

EX(3) RCT H 807638-73-7

STAGE(1)
 RCT D 584-08-7 K2CO3
 SOL 75-03-8 MeCN
 CON -5 deg C
 STAGE(2)
 RCT A 152922-73-1
 SOL 75-03-8 MeCN

L3 ANSWER 5 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

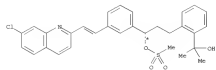
STAGE(2)

RCT B 162489-71-6
 SOL 1029-89-9 THF
 CON SUBSTAGE(1) -10 - -5 deg C
 SUBSTAGE(2) 8 hours, -5 deg C

PRO U 1000788-71-5

EX(9) OF 14 COMPOUND OF EX(3), EX(4)

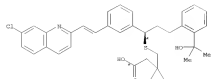
EX(9) H + A ==> L



H



A

2
STEPS →

L

EX(3) RCT H 807638-73-7

L3 ANSWER 5 OF 16 CASREACT COPYRIGHT 2009 ACS on STM (Continued)

STAGE(1)

RCT D 584-08-1 K2CO3

SOL 75-55-8 MeOH

CON -5 deg C

STAGE(2)

RCT A 153922-73-1

SOL 75-55-8 MeOH

CON SUBSTANCE(1) 15 minutes, -5 - 0 deg C

SUBSTANCE(2) 0 deg C -> 20 deg C

SUBSTANCE(3) 16 hours, 20 - 25 deg C

PRO F 855473-51-7

XX(14)

RCT F 855473-51-7

RCT M 1310-73-2 NaOH

PRO L 158946-92-8

SOL 129-99-9 THF, 67-56-1 MeOH, 7732-18-5 Water

CON SUBSTANCE(1) room temperature -> 0 deg C

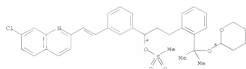
SUBSTANCE(2) 2 days, room temperature

XX(12) OF 14 COMPOSED OF XX(6), XX(7)

XX(12) 7 + 8 ==> L



7



8

L3 ANSWER 6 OF 16 CASREACT COPYRIGHT 2009 ACS on STM

ACCESSION NUMBER:

TITLE

Process for preparation of 1-(necroptonyl)cyclopropanecarboxylic acid

INVENTOR(S):

PATENT ASSIGNER(S):

SOURCE:

DOCUMENT TYPE:

LANGUAGE:

FAMILY AC. NUM. COUNTRY:

PATENT INFORMATION:

Joseph

Chambers Ltd., Israel

RCT Int. Appl., 19pp.

COBOL: P1X33

Patent

English

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L3 ANSWER 5 OF 16 CASREACT COPYRIGHT 2009 ACS on STM (Continued)

STAGE(1)

RCT V 109-72-8 EtOH

SOL 109-99-9 THF

CON SUBSTANCE(1) 25 - 30 deg C

SUBSTANCE(2) 20 deg C -> -15 deg C

SUBSTANCE(3) 30 minutes, -5 deg C

STAGE(2)

RCT B 162489-71-6

SOL 109-99-9 THF

CON SUBSTANCE(1) -10 - -5 deg C

SUBSTANCE(2) 8 hours, -5 deg C

PRO U 1000700-71-5

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(16)

RCT V 109-72-8 EtOH

SOL 109-99-9 THF

CON SUBSTANCE(1) 25 - 30 deg C

SUBSTANCE(2) 20 deg C -> -15 deg C

SUBSTANCE(3) 30 minutes, -5 deg C

STAGE(2)

RCT B 162489-71-6

SOL 109-99-9 THF

CON SUBSTANCE(1) -10 - -5 deg C

SUBSTANCE(2) 8 hours, -5 deg C

PRO U 1000700-71-5

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(17)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(18)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(19)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(20)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(21)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(22)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(23)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(24)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(25)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(26)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(27)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(28)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(29)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(30)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(31)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(32)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(33)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(34)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(35)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(36)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(37)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(38)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature -> 60 deg C

SUBSTANCE(2) 12 hours, 60 deg C

XX(39)

RCT U 1000700-71-5

RCT W 24057-80-1 pyridinium tosylate

PRO L 158946-92-8

SOL 109-99-9 THF, 67-56-1 MeOH

CON SUBSTANCE(1) room temperature

02/18/2009

10-576,971.trn

L3 ANSWER 6 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

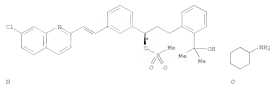
SOL 141-79-6 AcOEt
CON 25 deg C

PRO P 945934-73-6

RX(7) OF 10 COMPOSED OF RX(3), RX(4)
RX(7) G + N + O ==> P

● H2C

G

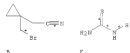


H

P1 CH 1
YIELD 65%

L3 ANSWER 6 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

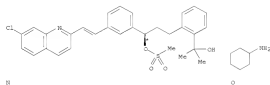
RX(9) B + F + N + O ==> P



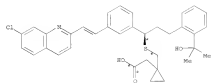
B



F

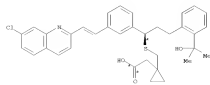


H

P1 CH 1
YIELD 65%P1 CH 2
YIELD 65%RX(2) RCT B 536593-69-4, F 62-56-6
PRO G 945934-71-7

Page 22

L3 ANSWER 6 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

P1 CH 2
YIELD 65%

RX(3) RCT G 945934-74-7

STAGE(1)

RCT J 1310-73-2 MeOH

SOL 7732-18-5 Water

CON SUBSTAGE(1) 14 hours, room temperature -> reflux

SUBSTAGE(2) reflux -> room temperature

STAGE(2)

RCT K 64-18-6 BOC2H

SOL 141-79-6 AcOEt

CON -5 - 5 deg C, pH 3.5 - 4

PRO I 162515-68-6

RX(4) RCT I 162515-68-6

STAGE(1)

RCT J 1310-73-2 MeOH

SOL 68-12-2 DMF, 7732-18-5 Water

CON 10 minutes, room temperature

STAGE(2)

RCT H 920739-17-9

SOL 105-89-9 THF

CON 2 hours, 25 deg C

STAGE(3)

RCT O 108-91-8

SOL 141-79-6 AcOEt

CON 25 deg C

PRO P 945934-73-6

RX(9) OF 10 COMPOSED OF RX(2), RX(3), RX(4)

L3 ANSWER 6 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

SOL 67-64-1 Me2CO

CON SUBSTAGE(1) 15 hours, room temperature -> reflux

SUBSTAGE(2) reflux -> -3 deg C

SUBSTAGE(3) 1 hour

RX(3) RCT G 945934-74-7

STAGE(1)

RCT J 1310-73-2 MeOH

SOL 7732-18-5 Water

CON SUBSTAGE(1) 14 hours, room temperature -> reflux

SUBSTAGE(2) reflux -> room temperature

STAGE(2)

RCT K 64-18-6 BOC2H

SOL 141-79-6 AcOEt

CON -5 - 5 deg C, pH 3.5 - 4

PRO I 162515-68-6

RX(4) RCT I 162515-68-6

STAGE(1)

RCT J 1310-73-2 MeOH

SOL 68-12-2 DMF, 7732-18-5 Water

CON 10 minutes, room temperature

STAGE(2)

RCT H 920739-17-9

SOL 105-89-9 THF

CON 2 hours, 25 deg C

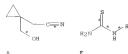
STAGE(3)

RCT O 108-91-8

SOL 141-79-6 AcOEt

CON 25 deg C

PRO P 945934-73-6

RX(10) OF 10 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
RX(10) A + F + N + O ==> P

A

F

02/18/2009

10-576,971.trn

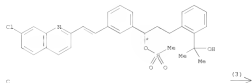
L3 ANSWER 7 OF 16 CASREACT COPYRIGHT 2009 ACS on STM (Continued)
 PRO D 942303-94-0
 RTE alternative preparation shown

RX(1) OF 4 A + D + C ==> X



A

D

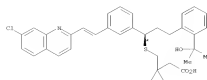


C



X: CH 1

L3 ANSWER 7 OF 16 CASREACT COPYRIGHT 2009 ACS on STM (Continued)



X: CH 2

RX(7) RCT A 162515-68-6, J 108-68-5

STAGE(1)

SOL 109-99-9 THF
 COB 109-99-9 2 hours, 25 deg C
 SUBSTAGE(2) 25 deg C -> -40 deg C

STAGE(2)

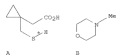
RCT E 109-72-8 Pd/L
 COB 70 minutes, -40 - -20 deg C

STAGE(3)

RCT C 807638-71-7
 SOL 109-99-9 THF
 COB 12 hours, -10 - -5 deg C

PRO E 942303-98-2
 RTE alternative preparation shown

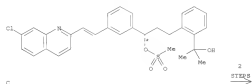
RX(1) OF 4 COMPOSED OF RX(1), RX(2)
 RX(4) A + B + C ==> G



A

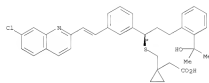
B

L3 ANSWER 7 OF 16 CASREACT COPYRIGHT 2009 ACS on STM (Continued)



C

2
 STAGE



● Ba

G
 YIELD 90%

RX(1) RCT A 162515-68-6, B 109-02-4

STAGE(1)

SOL 109-99-9 THF
 COB 109-99-9 2 hours, 25 deg C
 SUBSTAGE(2) 25 deg C -> -40 deg C

STAGE(2)

RCT E 109-72-8 Pd/L
 COB 30 minutes, -40 - -20 deg C

STAGE(3)

RCT C 807638-71-7
 SOL 109-99-9 THF
 COB 12 hours, -10 - -5 deg C

PRO D 942303-94-0
 RTE alternative preparation shown

RX(2) RCT D 942303-98-0
 RCT B 124-41-4 NaOMe

L3 ANSWER 7 OF 16 CASREACT COPYRIGHT 2009 ACS on STM (Continued)

PRO G 151761-02-1
 SOL 108-68-5 THF
 COB 30 minutes, 25 - 30 deg C

L3 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)

STAGE(1)
 RCT E 67-69-5 IMBO, F 124-61-4 NaOMe
 SOL 67-66-3 MeOH
 CON Low temperature -> 0 deg C

STAGE(2)
 RCT A 162515-68-6
 CON 60 minutes, -5 - 0 deg C

STAGE(3)
 RCT B 929739-17-9
 CON SUBSTAGE(1) -5 - 0 deg C
 SUBSTAGE(1) 12 hours, -5 - 5 deg C

STAGE(4)
 SOL 7732-18-5 Water
 CON 30 minutes, 10 - 20 deg C

STAGE(5)
 RCT D 1310-73-2 NaOH
 SOL 7732-18-5 Water
 CON 10 - 20 deg C

STAGE(6)
 RCT C 151-83-1
 SOL 142-70-4 MeOH
 CON 10 hours, 25 - 35 deg C

PRO D 577933-88-9
 RTE alternative preparation shown

EX(2) RCT D 577933-88-9
 RCT F 124-61-4 NaOMe
 PRO K 151767-92-1
 SOL 67-66-3 MeOH
 CON 60 minutes, 25 - 35 deg C

L3 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN

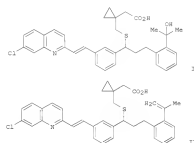
ACCESSION NUMBER: 1461162515 CASREACT
 TITLE: Purification of Montelukast
 SUBSTOR(5): Steinhausen, Gertay, Shapiro, Kossygi, Chen, Kuhn
 PATENT ASSIGNEE(S): Teva Pharmaceutical Industries Ltd., Israel; Teva
 Pharmaceutical Usa, Inc.
 SOURCE: PCT Int. Appl., 34pp.
 COUNTRY: ISRAEL
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006005865	A1	20060111	WO 2006-0256192	20060705
WI, ME, AU, BR, CA, CN, DE, DK, EP, ES, FI, FR, GB, GR, HU, IL, IN, JP, KR, MA, MX, MY, NZ, PL, PT, RU, SG, SI, SK, TH, TR, TW, UA, US, VE, VN, ZA, ZM, ZW				
CA 2608369	A1	20070111	CA 2006-060363	20060705
US 20070078158	A1	20070405	US 2006-481877	20060705
EP 1594448	A1	20060402	EP 2006-78639	20060705
JP 2007004100	T	20060410	JP 2007-530314	20060705
MX 2007002629	A	20060328	MX 2007-3409	20060705
BR 2007008504	A	20070829	BR 2007-765147	20070105
AR 2007009374	A	20080111	AR 2007-080706	20071004
IN 10131317	A	20080702	IN 2006-06014290	20080602
RU 2007013386	A	20070621	RU 2005-760703	20060613
US 2005-079006			US 2005-079006	20050705
WO 2006-0256192			WO 2006-0256192	20060705
EP 2007-765147			EP 2007-765147	20070105

PRIORITY AFFILI. INFO.

GI

L3 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)

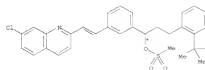


AB The present invention provides methods of purifying Montelukast (I), a new isolated impurity of Montelukast of formula (II), method for its isolation, and method of using Montelukast impurity as a reference marker and a reference standard. A process for preparing pure Montelukast sodium salt comprises (1) providing a Montelukast free acid, (2) converting the Montelukast free acid to the di-n-propylamine Montelukast salt, (3) and converting the di-n-propylamine Montelukast salt to Montelukast sodium salt. The impurity is used as a reference marker for determination of the purity of Montelukast.

By NPL See Ref. 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

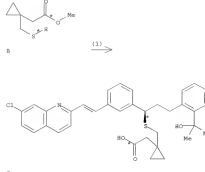
FORMAT

EX(1) OF 13 A + B ==> C...



A

L3 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)



EX(1) RCT A 807638-71-7, B 152922-73-1

STAGE(1)
 RCT D 1310-73-2 NaOH
 SOL 7732-18-5 Water, 127-18-5 AcOH
 CON SUBSTAGE(1) 9 minutes, -7 deg C
 SUBSTAGE(2) -7 deg C -> -5 deg C
 SUBSTAGE(3) 1 hour, -6 deg C
 SUBSTAGE(4) 1.5 hours, 10 deg C
 SUBSTAGE(5) 18 deg C -> 38 deg C
 SUBSTAGE(6) 1 hour, 38 deg C

STAGE(2)
 RCT D 1310-73-2 NaOH
 SOL 7732-18-5 Water
 CON overnight, 38 deg C

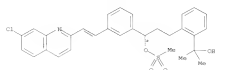
STAGE(3)
 RCT E 7647-14-5 HCl
 SOL 7732-18-5 Water

STAGE(4)
 RCT F 67-69-4 L-(+)-Tartaric acid
 SOL 109-99-9 THF
 CON pH 3 - 5

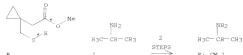
PRO C 159646-92-8

EX(4) OF 13 COMPOUND OF EX(1), EX(2)

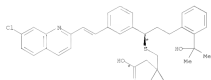
13 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)



A



B

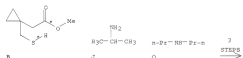


B; CN 2

RX(1) NCT A 807638-71-7, B 352922-73-3

STAGE(1)
 RTT D 1310-73-2 NaOH
 SOL 7732-18-5 Water, 127-19-5 AcOH
 CON SUBSTAGE(1) 3 minutes, -7 deg C
 SUBSTAGE(2) -7 deg C -> -3 deg C
 SUBSTAGE(3) 1 hour, -6 deg C
 SUBSTAGE(4) 2.5 hours, 18 deg C

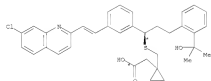
13 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)



B

n-Pr-CH=CH-Pr-n

B; CN 1



B; CN 2

RX(1) NCT A 807638-71-7, B 352922-73-3

STAGE(1)
 RTT D 1310-73-2 NaOH
 SOL 7732-18-5 Water, 127-19-5 AcOH
 CON SUBSTAGE(1) 3 minutes, -7 deg C
 SUBSTAGE(2) -7 deg C -> -3 deg C
 SUBSTAGE(3) 1 hour, -6 deg C
 SUBSTAGE(4) 2.5 hours, 18 deg C
 SUBSTAGE(5) 18 deg C -> 28 deg C
 SUBSTAGE(6) 1 hour, 38 deg C

STAGE(2)
 RTT D 1310-73-2 NaOH
 SOL 7732-18-5 Water
 CON overnight, 38 deg C

STAGE(3)
 RTT E 7647-14-5 NaCl
 SOL 7732-18-5 Water

STAGE(4)
 RTT F 87-69-4 L-(+)-Tartaric acid
 SOL 109-99-9 THF

13 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)

STAGE(2)
 RTT D 1310-73-2 NaOH
 SOL 7732-18-5 Water
 CON overnight, 38 deg C

STAGE(3)
 RTT E 7647-14-5 NaCl
 SOL 7732-18-5 Water

STAGE(4)
 RTT F 87-69-4 L-(+)-Tartaric acid
 SOL 109-99-9 THF
 CON pH 3 - 5

PRO C 158966-92-8

RX(2) NCT C 158966-92-8, J 75-73-0

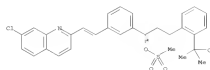
STAGE(1)
 CON SUBSTAGE(1) 0.5 hours, room temperature
 SUBSTAGE(2) 55 deg C, 20 mbar

STAGE(2)
 RTT L 78-33-3 EtOAc
 CON 50 deg C

PRO K 918972-53-9

RX(10) OF 13 COMPOSED OF RX(1), RX(2), RX(4)

RX(10) A + B + J + Q -> E



A

13 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)

PRO C 158966-92-8

RX(2) NCT C 158966-92-8, J 75-73-0

STAGE(1)
 CON SUBSTAGE(1) 0.5 hours, room temperature
 SUBSTAGE(2) 55 deg C, 20 mbar

STAGE(2)
 RTT L 78-33-3 EtOAc
 CON 50 deg C

PRO K 918972-53-9

RX(4) NCT K 918972-53-9

STAGE(1)
 RTT B 64-19-7 AcOH
 SOL 109-99-9 THF, 108-88-3 PhMe
 CON 40 minutes, room temperature, pH 5 - 6

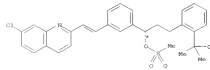
STAGE(2)
 RTT Q 142-84-7
 CON 0.5 hours, room temperature

STAGE(3)
 RTT T 108-88-3 PhMe
 CON SUBSTAGE(1) 40 deg C
 SUBSTAGE(2) 40 deg C -> 25 deg C
 SUBSTAGE(3) 0.5 hours, 25 deg C
 SUBSTAGE(4) 25 deg C -> 5 deg C
 SUBSTAGE(5) overnight, 0 deg C

PRO X 880769-26-6

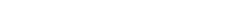
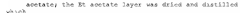
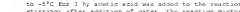
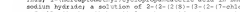
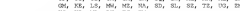
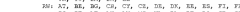
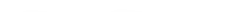
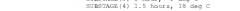
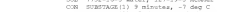
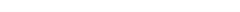
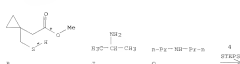
RX(13) OF 13 COMPOSED OF RX(2), RX(3), RX(4), RX(5)

RX(13) A + B + J + Q -> E



A

L3 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)



L3 ANSWER 9 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)

STAGE(4)

REF F 87-49-4 L-(+)-Tartaric acid

SOL 109-99-9 THF

CON pH 3 - 5

PRO C 158966-92-8

RX(2) ACT C 158966-92-8, J 75-73-0

STAGE(1)

SUBSTAGE(1) 0.5 hours, room temperature

SUBSTAGE(2) 55 deg C, 20 mbar

STAGE(2)

REF J 75-93-3 EtOAc

CON 50 deg C

PRO K 918972-53-9

RX(4) ACT K 918972-53-9

STAGE(1)

REF S 44-19-7 AcOH

SOL 109-99-9 THF, 100-88-3 DMAc

CON 40 minutes, room temperature, pH 5 - 6

STAGE(2)

REF Q 142-84-7

CON 0.5 hours, room temperature

STAGE(3)

REF T 100-88-3 DMAc

CON SUBSTAGE(1) 40 deg C

SUBSTAGE(2) 40 deg C -> 25 deg C

SUBSTAGE(3) 0.5 hours, 25 deg C

SUBSTAGE(4) 25 deg C -> 0 deg C

SUBSTAGE(5) overnight, 0 deg C

PRO E 880769-26-6

RX(15) ACT E 880769-26-6

REF V 861-45-5 NaCNu-t

PRO U 151747-02-3

SOL 100-88-3 DMAc

CON SUBSTAGE(1) 30 minutes, room temperature

SUBSTAGE(2) 30 minutes, 30 - 40 deg C

RX(1) ACT A 907638-71-7, B 132922-73-3

STAGE(1)

REF D 1310-73-2 NaOH

SOL 7732-18-5 Water, 127-19-5 AcOH

CON SUBSTAGE(1) 3 minutes, -7 deg C

SUBSTAGE(2) -7 deg C -> -1 deg C

SUBSTAGE(3) 1 hour, -6 deg C

SUBSTAGE(4) 1.5 hours, 18 deg C

SUBSTAGE(5) 18 deg C -> 38 deg C

02/18/2009

10-576,971.trn

L3 ANSWER 10 OF 16 CASRACT COPYRIGHT 2009 ACS ON STM (Continued)

SOL 109-99-9 THF, 67-68-5 DMGSO
CON SUBSTAGE(1) 1.5 hours, -5 - 0 deg C
SUBSTAGE(2) 1 hour, 0 - 5 deg C

STAGE(3)
NOT E 7732-18-5 Water, F 64-19-7 AcOH
CON 30 minutes, -5 - 0 deg C

STAGE(4)
NOT G 7786-30-3 MgCl2
SOL 67-68-1 MeOH, 141-78-6 AcOEt
CON 30 minutes, 25 - 30 deg C

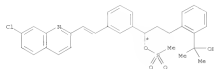
STAGE(5)
SOL 108-20-3 Isopropyl ether
CON cooled

PRO C 577953-86-7
NTE stereoselective

EX(12) OF 4 A + B ==> C



A



B



L3 ANSWER 10 OF 16 CASRACT COPYRIGHT 2009 ACS ON STM (Continued)

SOL 109-99-9 THF, 67-68-5 DMGSO
CON SUBSTAGE(1) 1.5 hours, -5 - 0 deg C
SUBSTAGE(2) 1 hour, 0 - 5 deg C

STAGE(3)
NOT E 7732-18-5 Water, F 64-19-7 AcOH
CON 30 minutes, -5 - 0 deg C

STAGE(4)
NOT G 7786-30-3 MgCl2
SOL 67-68-1 MeOH, 141-78-6 AcOEt
CON 30 minutes, 25 - 30 deg C

STAGE(5)
SOL 108-20-3 Isopropyl ether
CON cooled

PRO C 577953-86-7
NTE stereoselective

C

EX(12) NCT A 162555-68-6

STAGE(1)
NOT H 109-72-8 BuLi
SOL 109-99-9 THF
CON 2 hours, -15 - -10 deg C

STAGE(2)
NOT B 807438-71-7
SOL 109-99-9 THF
CON SUBSTAGE(1) 2 hours, -5 - 0 deg C
SUBSTAGE(2) 15 hours, -5 - 0 deg C

STAGE(3)
NOT H 7647-14-5 HAcCl
SOL 7732-18-5 Water
CON <0 deg C

STAGE(4)
NOT G 7786-30-3 MgCl2
SOL 67-68-1 MeOH, 141-78-6 AcOEt
CON 30 minutes, 25 - 30 deg C

STAGE(5)
SOL 108-20-3 Isopropyl ether
CON cooled

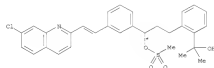
PRO C 577953-86-7
NTE stereoselective

EX(13) OF 4 A + B ==> G

L3 ANSWER 10 OF 16 CASRACT COPYRIGHT 2009 ACS ON STM (Continued)



A



B



L3 ANSWER 10 OF 16 CASRACT COPYRIGHT 2009 ACS ON STM (Continued)

SOL 109-99-9 THF, 67-68-5 DMGSO
CON SUBSTAGE(1) 2 hours, -5 - 0 deg C
SUBSTAGE(2) 15 hours, -5 - 0 deg C

STAGE(3)
NOT H 7647-14-5 HAcCl
SOL 7732-18-5 Water
CON <0 deg C

STAGE(4)
NOT F 10043-52-4 CuCl2
SOL 67-68-1 MeOH, 141-78-6 AcOEt
CON 30 minutes, 25 - 30 deg C

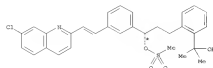
STAGE(5)
SOL 108-20-3 Isopropyl ether
CON cooled

PRO C 577953-85-6
NTE stereoselective

EX(4) OF 4 A + B ==> Q



A



B



EX(13) NCT A 162555-68-6

STAGE(1)
NOT H 109-72-8 BuLi
SOL 109-99-9 THF
CON 2 hours, -15 - -10 deg C

STAGE(2)
NOT B 807438-71-7
SOL 109-99-9 THF

L3 ANSWER 11 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

STAGE(2)

REX 2 7647-14-5 NaCl
 SOL 7732-18-5 Water, 100-21-6 Acetic acid, 1-methylethyl ester
 CON 15 minutes, heated

STAGE(3)

ROT 1 1712-73-2 NaOH
 SOL 7732-18-5 Water, 64-17-8 EtOH

PRO N 151767-02-5

REX small molecule stage 2, author shows purification, optimization
 study, soluble, stereoselective

L3 ANSWER 12 OF 16 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:

143156935 CASREACT

TITLE:

Promote for the preparation of
 [6-(6-[[1-[1-[2-(17-cyano-2-
 quinolinyl)ethenyl]phenyl]-3-[2-
 1-hydroxy-3-

methylethyl)phenyl]propyl]thio]methyl]cyclopropanecarbox-
 ic acid (montelukast) and its pharmaceutically
 acceptable salts

INVENTOR(S):

Sundaram, Venkataraman; Rajan, Sriniwas; Thirumalai,
 Rulana; Venkata Naga Chandra Sekhar; Srivastava,
 Anil Kumar; Rastogi, Anil; Pandey, Anvula; Rajasekhar

PATENT ASSIGNEE(S):

India
 U.S. Pat. Appl. Publ., 7 pp.

SOURCE:

CORREL: US2000

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050234241	A1	20051029	US 2004-921562	20040902
US 7129653	B2	20070315		
IN 20040402042	A	20070314	IN 2004-CET42	20040415
IN 2004-CET42			IN 2004-CET42	20040415

PRIORITY APPL. INFO.:

CI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention is related to a process for preparing montelukast
 (2)

Involving substitution of 11 (preparation given) with an alkali salt of a
 compound of formula III (wherein 2oCH or COME2 followed by hydrolysis.

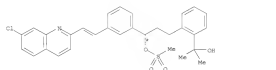
REFERENCE COUNT: 3 THREE ARE CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

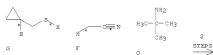
RX(12) OF 31 COMPOSED OF RX(2), RX(3)

RX(13) C + O + F + O ==> F

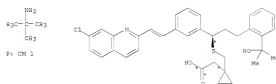
L3 ANSWER 12 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



C



G



Pr: CH 1

Pr: CH 2

RX(12) ROT C 807698-71-7, G 5617-79-8, F 75-05-8

STAGE(1)

ROT 1 109-72-8 India
 SOL 68-12-3 DMF, 100-54-3 Benzene
 CON 6 - 8 hours, -25 - -10 deg C

STAGE(2)

ROT 2 7647-14-5 NaCl
 SOL 100-89-3 EtOH, 7732-18-5 Water
 CON 20 minutes

STAGE(3)

SOL 7732-18-5 Water, 64-17-8 EtOH
 CON 30 - 40 minutes, 25 - 35 deg C

L3 ANSWER 12 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

PRO N 866923-62-8

REX stereoselective

RX(13) ROT N 866923-62-8

STAGE(1)

CON 6 - 8 hours, 110 - 122 deg C

STAGE(2)

SOL 100-89-3 EtOH, 7732-18-5 Water
 CON 20 - 30 minutes, 90 deg C

STAGE(3)

ROT N 64-19-7 AcOH
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2
 CON 25 - 35 deg C, pH 4.8 - 5

STAGE(4)

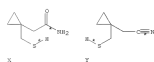
ROT O 75-64-9
 SOL 67-64-1 Me2CO
 CON 8 - 10 hours, 25 - 35 deg C

PRO F 851755-58-3

REX anionic lyx added stage 1

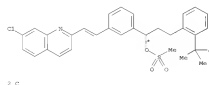
RX(15) OF 31 COMPOSED OF RX(6), RX(7)

RX(15) X + Y + 2 C ==> AA



X

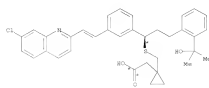
Y



2 C

2
STEP2

L3 ANSWER 12 OF 16 CASRACT COPYRIGHT 2009 ACS ON STN (Continued)



AA

RX(16) RCT X 162515-69-7, Y 866923-64-0

STAGE(1)
 RGT 1 109-72-8 BuLi
 SOL 68-12-2 DMF, 110-54-3 Benzene
 COH 10 minutes, <0 deg C

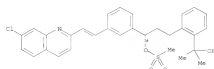
STAGE(2)
 RCT C 807638-71-7
 COH 5 hours, <0 deg C

PRO Z 866923-63-9
 RTE stereoselective

RX(17) RCT Z 866923-63-9
 RGT 5 1310-58-3 KOH
 PRO AA 152922-12-0
 SOL 111-46-6 (HOC6H2CH2)2O, 7732-18-5 Water
 COH 24 hours, reflux

RX(22) OF 31 COMPOSED OF RX(12), RX(13), RX(15)

RX(22) C + G + F + O ==> U



C

L3 ANSWER 12 OF 16 CASRACT COPYRIGHT 2009 ACS ON STN (Continued)

STAGE(1)
 COH 8 hours, 118 - 122 deg C

STAGE(2)
 SOL 108-88-3 THF, 7732-18-5 Water
 COH 30 - 30 minutes, 90 deg C

STAGE(3)
 RGT H 64-19-7 AcOH
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2
 COH 25 - 35 deg C, pH 4.8 - 5

STAGE(4)
 RCT O 75-64-9
 SOL 67-66-1 Me2CO
 COH 8 - 10 hours, 25 - 35 deg C

PRO F 851755-58-3
 RTE exsiccative 1st added stage 1

RX(15) RCT F 851755-58-3

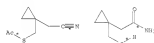
STAGE(1)
 RGT H 64-19-7 AcOH
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2
 COH 30 - 60 minutes, 25 - 35 deg C

STAGE(2)
 RGT V 1310-73-2 NaOH
 SOL 67-66-1 Me2CO
 COH 30 - 60 minutes, 25 - 35 deg C

PRO U 152767-02-1
 RTE work-up

RX(24) OF 33 COMPOSED OF RX(19), RX(16), RX(17)

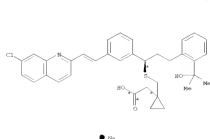
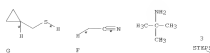
RX(24) AB + X + 2 C ==> AA



AB

X

L3 ANSWER 12 OF 16 CASRACT COPYRIGHT 2009 ACS ON STN (Continued)



U

RX(2) RCT C 807638-71-7, G 1617-78-8, F 75-05-0

STAGE(1)
 RGT 1 109-72-8 BuLi
 SOL 68-12-2 DMF, 110-54-3 Benzene
 COH 6 - 8 hours, -15 - -10 deg C

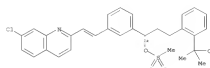
STAGE(2)
 RGT J 7647-14-5 HCl
 SOL 108-88-3 THF, 7732-18-5 Water
 COH 20 minutes

STAGE(3)
 RGT 7732-18-5 Water, 64-19-7 AcOH
 COH 30 - 40 minutes, 25 - 35 deg C

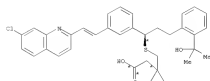
PRO H 866923-62-8
 RTE stereoselective

RX(17) RCT H 866923-62-8

L3 ANSWER 12 OF 16 CASRACT COPYRIGHT 2009 ACS ON STN (Continued)



2 C



AA

RX(19) RCT AB 152922-12-0

STAGE(1)
 RGT AC 124-41-4 HAcOH
 SOL 67-66-1 Me2CO
 COH -15 - -12 deg C

STAGE(2)
 RGT H 64-19-7 AcOH
 SOL 7732-18-5 Water
 COH 20 - 30 minutes, <0 deg C, acidify

PRO Y 866923-64-0

RX(16) RCT X 162515-69-7, Y 866923-64-0

STAGE(1)
 RGT 1 109-72-8 BuLi
 SOL 68-12-2 DMF, 110-54-3 Benzene
 COH 20 minutes, <0 deg C

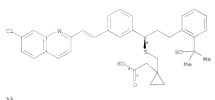
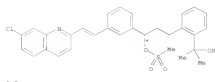
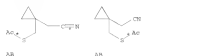
STAGE(2)
 RCT C 807638-71-7
 COH 5 hours, <0 deg C

PRO Z 866923-63-9

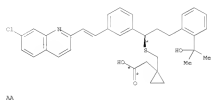
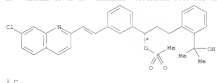
L3 ANSWER 12 OF 16 CASRACT COPYRIGHT 2009 ACS on STN (Continued)

EX(7) RCT S 866923-63-9
RUT S 1310-58-3 MOH
PRO AA 158964-92-8
SOL 111-46-4 (BOCHER2)20, 7732-18-5 Water
CON 24 hours, reflux
NTE chemoselective, 3,4-acetamidobenzonitrile

EX(12) OF 31 COMPOSED OF EX(10), EX(6), EX(7)
EX(12) 2 AB + 2 C ==> AA



L3 ANSWER 12 OF 16 CASRACT COPYRIGHT 2009 ACS on STN (Continued)



EX(9) RCT AB 152922-72-0

STAGE(1)
RUT AC 124-41-4 NaOMe
SOL 47-56-3 MeOH
CON -15 - +12 deg C
STAGE(2)
RUT H 64-29-7 AcOH
SOL 7732-18-5 Water
CON 20 - 30 minutes, <0 deg C, acidify
PRO Y 866923-64-0

EX(10) RCT AB 152922-72-0
RUT S 1310-58-3 MOH
PRO X 162515-69-7, Y 866923-64-0
SOL 67-56-3 MeOH, 7732-18-5 Water
CON 808708(1) room temperature
808708(2) <50 deg C
NTE chemoselective, 3,4-acetamidobenzonitrile

EX(6) RCT X 162515-69-7, Y 866923-64-0
STAGE(1)
RUT I 109-72-8 BuLi
SOL 68-12-2 DMF, 110-54-3 Benzene
CON 10 minutes, <0 deg C

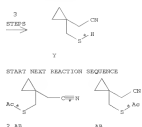
L3 ANSWER 12 OF 16 CASRACT COPYRIGHT 2009 ACS on STN (Continued)

EX(10) RCT AB 152922-72-0
RUT S 1310-58-3 MOH
PRO X 162515-69-7, Y 866923-64-0
SOL 67-56-3 MeOH, 7732-18-5 Water
CON 808708(1) room temperature
808708(2) <50 deg C
NTE chemoselective, 3,4-acetamidobenzonitrile

EX(6) RCT X 162515-69-7, Y 866923-64-0
STAGE(1)
RUT I 109-72-8 BuLi
SOL 68-12-2 DMF, 110-54-3 Benzene
CON 10 minutes, <0 deg C
STAGE(2)
RCT C 807638-71-7
CON 5 hours, <0 deg C
PRO S 866923-63-9
NTE stereoselective

EX(7) RCT S 866923-63-9
RUT S 1310-58-3 MOH
PRO AA 158964-92-8
SOL 111-46-4 (BOCHER2)20, 7732-18-5 Water
CON 24 hours, reflux

EX(30) OF 31 COMPOSED OF REACTION SEQUENCE EX(9), EX(6), EX(7)
AND REACTION SEQUENCE EX(10), EX(6), EX(7)
...AB ==> Y...
...2 AB + 2 C ==> AA



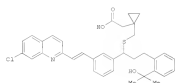
L3 ANSWER 12 OF 16 CASRACT COPYRIGHT 2009 ACS on STN (Continued)

EX(7) RCT S 866923-63-9
RUT S 1310-58-3 MOH
PRO AA 158964-92-8
SOL 111-46-4 (BOCHER2)20, 7732-18-5 Water
CON 24 hours, reflux
STAGE(1)
RUT C 807638-71-7
CON 5 hours, <0 deg C
PRO S 866923-63-9
NTE stereoselective
STAGE(2)
RCT S 866923-63-9
RUT S 1310-58-3 MOH
PRO AA 158964-92-8
SOL 111-46-4 (BOCHER2)20, 7732-18-5 Water
CON 24 hours, reflux

13 ANMER 13 OF CASAKBAT COPYRIGHT 2020 ACS ON 27N
ACCESSION NUMBER: 14238157 CASAKBAT
TITLE: An improved method for preparation of montelukast
4654
and sodium salt
INVENTOR(S): Suril, Ranjay Singh, Jyotsnar, Surin, Gurddeep Singh,
Taneer, Madan Pal, Mahendra, Naveen
PATENT APPLICANT(S): Mergem Laboratories Limited, India
SOCCL: PCT Int. Appl., 26 pp.
COMPU: FINDED
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY AC NUM COUNT: 1
PATENT INFORMATION:

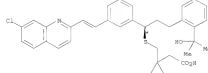
[illegible]

CA 2528228	AL	200412136	CA 2003-2528228	20030606
AU 2003253247	AL	200501014	AU 2003-253247	20030606
EP 1631550	AL	200603098	EP 2003-817134	20030606
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, NO, CY, TR, BG, CZ, EE, HU, SK				
US 20070082925	AL	20070412	US 2006-576971	20060425
ORITV APP18. INFO:			WO 2003-18214	20030606



A2 The invention relates to a preparation of montelukast acid sodium salt of formula I•Na in amorphous form, useful as leukotriene antagonist (no biol. data). The method comprises of following steps: (a) generating the

13 ANSWER 13 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



3. CM 2

806(2) 807 © 162515-68-6

```
STAGE(2)
NOT J 109-72-8 BuLi
SOL 109-39-9 THF, 110-54-3 Hexane
CON SUBSTAGE(2) -15 - -10 deg C
SUBSTAGE(2) 0.5 hours, -15 - -10 deg C
```

```
STAGE(2)
RCT C 807628-71-7
SOL 109-99-9 THF
CON SUBSTAGE(1) room temperature => -5 deg C
SUBSTAGE(2) -10 - -5 deg C
SUBSTAGE(3) 0.25 hours, -10 - -5 deg C
```

```
STAGE(3)
SOL 109-99-9 TEF
CON SUBSTAGE(1) 0.5 hours, -7 - -3 deg C
SUBSTAGE(2) 12 hours
```

STAGE(4)
RGT K 7647-24-5 NaCl
SW. 7782-28-4 Water

```
STAGE(5)
ACT 8 101-83-7
SOL 141-79-6 AcOEt
CON SUBSTAGE(1) 0.5 hours, 25 - 35 deg C
SUBSTAGE(2) 0.5 hours, 25 - 35 deg C
```

DOI: 10.1002/anie.200525134

EX(5) OF 6 COMPOSED OF EX(2), EX(3)

$$G + C + H$$

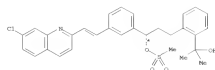
1.3 ANSWER 13 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)
dilithium dianion of 1-(mercaptomethyl)cyclopropane acetic acid by reacting with alkyl lithium, (b) coupling the acid dianion with wet methylate to get montelukast acid in crude form, (c) obtaining DCM salt

crude form by adding dicyclohexylamine (DCHA) to crude acid obtained in the above step (b), (d) purifying and converting the said DCHA salt in turn to the free acid by adding a strong acid, (e) dissolving the said free montelukast acid in a polar protic solvent with a source of sodium ions followed by evap. of the solvent and triturating of the residue with non-polar water immiscible solvent. For instance, 10% was obtained in the above prep. of 100 g of 100% pure 100% pure 100% pure 90-78% HPLC purity was 99.42%). The invention proposes industrially feasible and cost-effective process for high-yield and high-purity prepn. of

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

$$\text{Fe(2) OP 6} \quad \dots G + C + B \implies I \dots$$


5



3

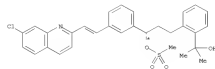


I

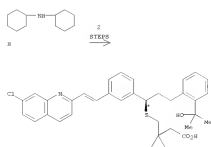
1.3 ANSWER 13 OF 16 CASEACT COPYRIGHT 2009 ACS on STN (Continued)



5



5



3

FOI(2) FCIT G 162515-68-6

```
STAGE(1)
EGF J 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON SURSTAGE(1) -15 - -10 deg C
```

L3 ANSWER 13 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

STAGE(2)
 NCT C 807638-71-7
 SOL 129-89-9 THEO
 CON SUBSTANCE(1) room temperature -> -5 deg C
 SUBSTANCE(2) -10 - -5 deg C
 SUBSTANCE(3) 0.25 hours, -10 - -5 deg C

STAGE(3)
 SOL 129-89-9 THEO
 CON SUBSTANCE(1) 0.5 hours, -7 - -3 deg C
 SUBSTANCE(2) 12 hours

STAGE(4)
 NCT E 7647-14-5 NaCl
 SOL 7732-10-5 Water

STAGE(5)
 NCT B 121-83-7
 SOL 141-79-6 AcOH
 CON SUBSTANCE(1) 0.5 hours, 25 - 35 deg C
 SUBSTANCE(2) 0.5 hours, 25 - 35 deg C

PRO I 577353-88-9

EX(2)
 NCT I 577353-88-9
 NCT Q 64-13-7 AcOH
 PRO I 577353-88-9
 SOL 7732-10-5 Water, 108-88-3 H₂O
 CON SUBSTANCE(1) 30 minutes, 25 - 35 deg C
 SUBSTANCE(2) 15 minutes, 25 - 35 deg C

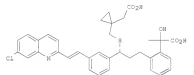
L3 ANSWER 14 OF 16 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 129-254909 CASREACT
 TITLE: Quinolone diacid derivatives, and preparation thereof,
 for leukotriene antagonist
 INVENTOR(S): Arison, Byron R.; Balasub, Suresh K.; Baillie, Thomas A.; Dufresne, Claude
 PATENT ASSIGNEE(S): Merck & Co., Inc.; 955; Merck Frost Canada Inc.
 SOURCE: ICT Int. Appl., 42 pp.
 CUBERI FIGURE
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY NO., NUM. COPY: 1
 PATENT INFORMATION(S):

PATIENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9803970	A1	19980317	WO 1998-054609	19980710
W1	AL, AM, AN, AS, BA, BB, BC, BD, BF, BG, CA, CH, CO, CZ, DE, DK, DM, DO, DR, ES, FI, GB, GR, GU, HK, HU, IL, IN, JP, KE, KR, KZ, LG, LU, LV, LY, MA, MC, MD, ME, MG, MI, MN, MU, MV, MY, NZ, OM, OS, PA, PE, PG, PH, PI, PL, PT, RU, SA, SD, SE, SG, SI, SK, SL, SR, SS, SV, TH, TJ, TM, TR, TT, UA, UG, UY, US, UZ, VN, YU			
PRO	GB, GR, HU, IL, IN, JP, KR, KZ, LG, LU, LV, LY, MA, MC, MD, ME, MG, MI, MN, MU, MV, MY, NZ, OM, OS, PA, PE, PG, PH, PI, PL, PT, RU, SA, SD, SE, SG, SI, SK, SL, SR, SS, SV, TH, TJ, TM, TR, TT, UA, UG, UY, US, UZ, VN, YU			
CA 2287151	A1	19980317	CA 1998-0283161	19980310
CA 2287151	C	20000120		
AO 2867550	A	19980920	AO 1998-07509	19980710
AO 726210	B2	20001102		
UG 158247	A	19990914	UG 1998-07949	19980710
EP 971587	A1	20000219	EP 1998-912511	19980710
EP 971587	B1	20000208		
EE 3732	B1	20000417	EE 1999-006	19980710
JP 2000134660	T	20001031	JP 1998-079688	19980710
AT 317224	T	20000215	AT 1998-912511	19980710
RU 2256973	T3	20000716	RU 1998-912511	19980710
US 1997-00417P			US 1997-00417P	19970311
GB 1997-11050			GB 1997-11050	19970529
WO 1998-054609			WO 1998-054609	19980710

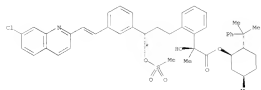
OTHER SOURCE(S): NAEPAT 129-254909
 GI

L3 ANSWER 14 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

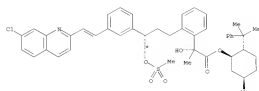


AB Compds. 1 are antagonists of the actions of leukotrienes. These compds. are useful as anti-asthmatic, anti-allergic, anti-inflammatory, and cytoprotective agents. They are also useful in treating angina, cerebral spasm, glomerular nephritis, hepatitis, endocarditis, urethritis, and allergic rejection. 1 are binary metabolites of montelukast sodium. Compound isolation and preparation are described.
 REFERENCE COPY: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE 36 FORMAT

EX(2) OF 48 ...2 K + D + E ==> L + H...

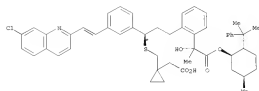


L3 ANSWER 14 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



5

(2)

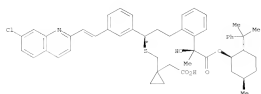


L

02/18/2009

10-576,971.trn

L3 ANSWER 14 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



M

RX(12) RCT K 162555-68-6

STAGE(1)

RUT R 109-72-8 BuLi

SOL 109-99-9 THF

STAGE(2)

RCT D 213380-30-4, K 213380-31-5

SOL 109-99-9 THF

STAGE(3)

RUT O 11125-02-9 NH4Cl

SOL 7732-18-5 Water

PRO L 213380-32-6, M 213380-33-7

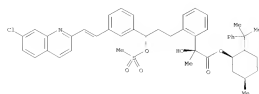
RX(13) OF 48 COMPOUND OF RX(12), RX(13)

RX(13) 2 M + D + E ==> 2 Q

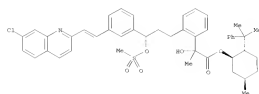


2 M

L3 ANSWER 14 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



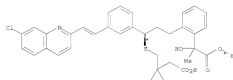
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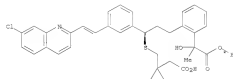
E

2
STEPS

L3 ANSWER 14 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



Q



Q

RX(12) RCT K 162555-68-6

STAGE(1)

RUT R 109-72-8 BuLi

SOL 109-99-9 THF

STAGE(2)

RCT D 213380-30-4, K 213380-31-5

SOL 109-99-9 THF

STAGE(3)

RUT O 11125-02-9 NH4Cl

SOL 7732-18-5 Water

PRO L 213380-32-6, M 213380-33-7

RX(13) RCT L 213380-32-6, M 213380-33-7

STAGE(1)

RUT R 1310-45-2 LiOH

SOL 64-17-5 EtOH, 7732-18-5 Water

STAGE(2)

RUT O 11125-02-9 NH4Cl, S 64-19-7 AcOH

SOL 7732-18-5 Water

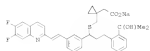
L3 ANSWER 14 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

PRO Q 213380-27-9

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10-576,971.trn

L3 ANSWER 15 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)
 ACCESSION NUMBER: 1261225193 CASREACT
 TITLE: The enantioselective synthesis of LTD4 antagonist L-705,738
 AUTHOR(S): Sudler, Daniel R.; Sager, Jose M.; Bergan, James J.;
 Mella, Kenneth M.; Bhupathy, M.; Volante, R. P.
 CORPORATE SOURCE: Process Research Department, Merck Research
 Laboratories, Rahway, NJ, 07065, USA
 SOURCE: Tetrahedron Asymmetry [1997], 8(1), 161-168
 CODEN: TASTET; EID: 9551-4166
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 CI



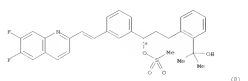
AB An efficient, 9-step synthesis of LTD4 antagonist L-705,738 sodium salt
 [1] was described. The syn. scheme was set via a chiral borane
 reduction.
 REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE PE
 FORMAT

PK(S) OF 36 ...A1 + AG ==> A2

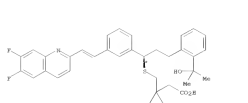


A1

L3 ANSWER 15 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)



A2



A3

PK(S) RCT A1 162515-68-6

STAGE(1)
 RCT AX 109-72-8 Bull
 SOL 109-99-3 TAP, 110-54-3 Benzene
 STAGE(2)
 RCT AG 188351-74-8
 STAGE(3)
 RCT P 64-19-7 AcOH
 SOL 7732-18-5 Water, 108-88-3 Pyridine
 STAGE(4)
 RCT AL 1310-73-2 NaOH
 PRO A2 152922-64-0

L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)
 ACCESSION NUMBER: 1271131787 CASREACT
 TITLE: Preparation of quinoline derivative leukotriene
 antagonists.

L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)
 ACCESSION NUMBER: 1271131787 CASREACT
 TITLE: Preparation of quinoline derivative leukotriene
 antagonists.

INVENTOR(S): Bhupathy, Mahadevan; McManis, James M.; Sudler,
 Daniel R.; Volante, Ralph P.; Bergan, James J.

PATENT ASSIGNMENT(S): March and Co., Inc., USA

SOURCE: PCT Int., Appl., 48 pp.
 CODEN: PTAED2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY RCT, NUM. COUNT: 1

PATENT INFORMATION:

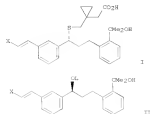
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WO 9518107	A1	19950706	WO 1994-021455	19941222
W1	NA, AU, BR, BG, BY, CA, CH, CN, DE, FI, GB, GR, HU, JP, KR, LA, LU, LV, MD, ME, MK, NL, NO, NZ, PL, PT, RU, SI, SK, TR, UA, US, VE, ES, AT, BE, CH, DE, DK, EE, ES, FR, GB, GR, IE, IT, LU, ME, NL, PT, SE, SF, BG, CF, CG, CI, CM, GA, GN, ML, NG, SN, TH, TD			
TM 416948	B	20010101	TM 1994-0311982	19941221
TM 446160	B	20010801	TM 2000-0311401	19941221
CA 2174607	A1	19950706	CA 1994-2179407	19941222
US 9514448	A	19950711	US 1995-14448	19941222
EP 686303	B2	19980205		
EP 737186	A1	19980106	EP 1995-006106	19941222
EP 737186	B1	19980819		
FI 917, BE, CH, DE, DK, EE, ES, FR, GB, GR, IE, IT, LU, NL, PT, SE				
CH 1138428	A	19970101	CH 1994-184671	19941221
CH 1046712	C	19931124		
JP 09507125	T	19970722	JP 1993-518152	19941222
JP 3640962	B2	20050420		
HU 76279	A2	19970728	HU 1996-1775	19941222
HU 226394	B1	20081129		
IN 2408452	A	19970801	IN 1994-4452	19941222
AZ 169906	AZ	19980915	AZ 1995-006106	19941222
EE 212534	T3	19981216	EE 1995-006106	19941222
CH 1138125	A	19980616	CH 1994-181515	19941222
CH 126807	C	20070718		
HU 2140909	G1	19991110	HU 1996-113796	19941222
CE 286079	BE	20000112	CE 1996-1878	19941222
PL 176671	PL	20000531	PL 1994-181515	19941222
HU 119018	B1	20040227	HU 1996-1312	19941222
HO 212539	C2	20040110	HO 1999-100900	19941222
CH 10101834	A	20071205	CH 2006-10091487	19941222
US 5416632	A	19970128	US 1994-139735	19950512
US 9602641	A	19960624	US 1996-1341	19960624
FI 113045	B1	20040227		
HU 1002049	A1	20000824	HU 1999-274062	19990302
US 6320052	US	20011120	US 1993-174921	19931229
LV 12113	B	19991110	US 1994-150462	19941229
US 1993-174921	US	20011120	US 1998-118791	19941222
US 1998-118791	US	20011120	US 1998-113796	19941222
WO 1994-0311982	WO	1994-0311982	WO 1994-0311982	19941222

PRIORITY APPL. INFO.:

02/18/2009

10-576,971.trn

L3 ANSWER 16 OF 16 CASBACK COPYRIGHT 2009 ACS ON STN (Continued)
 OTHER SOURCE(S): MARPAT 123:313787 US 1997-94368 19971008

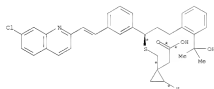
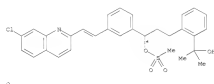


AB Totie oxazolid. [I, K = 7-chloroquinolin-2-yl, 6,7-difluoroquinolin-3-yl]
 or
 He salts thereof, were prepared by generating and reacting the dilithium
 dianion of 1-methoxyethyl-1-oxobut-2-ylidene with (II, I =
 was
 2-(2-[15]-[12-(17-chloro-2-quinolinyl)ethylphenyl]-1-
 methoxyethyl)propyl)phenyl-2-propanol (preparation given) and the
 nixture
 was aged 8.5 h at -5° to give 714 I (K = 7-chloroquinolin-2-yl),
 isolated as the dihydroxyamine salt.
 REFERENCE COUNT: 2 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
 FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE AS

RK(4) OF 28 ...L + O ==> P



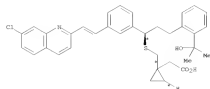
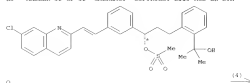
L3 ANSWER 16 OF 16 CASBACK COPYRIGHT 2009 ACS ON STN (Continued)



P, CH 2
YIELD 79%

RK(13) RCT K 169954-92-0
 RGT M 1310-72-2 NaOH
 PRO L 169954-92-1
 SOL 109-99-9 THF, 7732-18-5 Water

L3 ANSWER 16 OF 16 CASBACK COPYRIGHT 2009 ACS ON STN (Continued)



P, CH 2
YIELD 79%

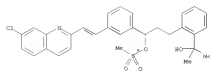
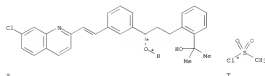
RK(4) RCT L 169954-92-1, O 169954-92-2
 RGT Q 109-72-8 BuLi
 PRO P 169954-94-3
 SOL 109-99-9 THF
 RTE -5°, 8.5 h

RK(10) OF 28 COMPOSED OF RK(3), RK(4)
 RK(10) K + O ==> P

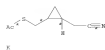
L3 ANSWER 16 OF 16 CASBACK COPYRIGHT 2009 ACS ON STN (Continued)

RK(4) RCT L 169954-92-1, O 169954-92-2
 RGT Q 109-72-8 BuLi
 PRO P 169954-94-3
 SOL 109-99-9 THF
 RTE -5°, 8.5 h

RK(17) OF 28 COMPOSED OF REACTION SEQUENCE RK(5), RK(4)
 AND REACTION SEQUENCE RK(3), RK(4)
 ...S + T ==> O...
 ...K + O ==> P



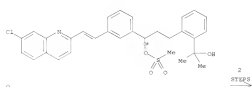
START NEXT REACTION SEQUENCE



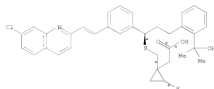
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L3 ANSWER 16 OF 16 CASRACT COPYRIGHT 2009 ACS on STN (Continued)



O

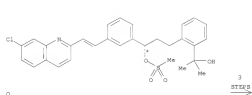
P: CH 3
YIELD 79%P: CH 2
YIELD 79%

KK(15) KCT B 142549-70-9, T 124-63-0
KCT D 10871-68-5 K1M (P-1)2
PRO O 169954-93-2
SOL 108-68-3 PhMe, 75-05-8 MeCN

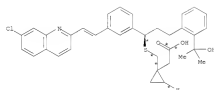
KK(13) KCT K 169954-92-0
KCT M 1310-73-2 MeOH
PRO L 169954-92-1
SOL 108-68-3 PhMe, 7732-18-5 Water

KK(14) KCT L 169954-92-1, O 169954-93-2

L3 ANSWER 16 OF 16 CASRACT COPYRIGHT 2009 ACS on STN (Continued)



O

P: CH 3
YIELD 79%P: CH 2
YIELD 79%

KK(15) KCT B 142549-70-9, T 124-63-0
KCT D 10871-68-5 K1M (P-1)2
PRO O 169954-93-2
SOL 108-68-3 PhMe, 75-05-8 MeCN

KK(14) KCT O 162902-71-9

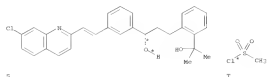
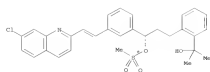
STAGE(1)
KCT W 1231-64-8 K1M, T 124-63-0 MeSO2C1
SOL 69-12-2 DMF, 108-68-3 PhMe

STAGE(2)
KCT V 507-09-5

L3 ANSWER 16 OF 16 CASRACT COPYRIGHT 2009 ACS on STN (Continued)

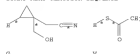
KCT Q 109-72-8 BuLi
PRO P 169954-94-3
SOL 109-69-8 THF
NTE -5*, 8.5 h

KK(16) OF 28 COMPOUND OF REACTION SEQUENCE KK(5), KK(14)
AND REACTION SEQUENCE KK(6), KK(7), KK(14)
...S + T ==> O...
...G + V + O ==> P

3
STEPS

O

START REACT REACTION SEQUENCE

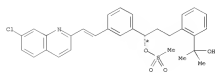
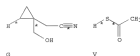


L3 ANSWER 16 OF 16 CASRACT COPYRIGHT 2009 ACS on STN (Continued)

PRO K 169954-91-0
KK(13) KCT K 169954-91-0
KCT M 1310-73-2 MeOH
PRO L 169954-92-3
SOL 108-68-3 PhMe, 7732-18-5 Water

KK(14) KCT L 169954-92-1, O 169954-93-2
KCT Q 109-72-8 BuLi
PRO P 169954-94-3
SOL 109-69-8 THF
NTE -5*, 8.5 h

KK(20) OF 28 COMPOUND OF KK(6), KK(13), KK(14)
KK(20) G + V + O ==> P



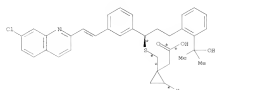
O

P: CH 3
YIELD 79%

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L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

F: CH 2
YIELD 79%

RX(16): NCT O 152922-71-9

STAGE(1)
RGT M 121-44-8 RL3N, T 124-63-0 MeSO2Cl
SOL 68-12-2 DMF, 108-88-3 PhMe

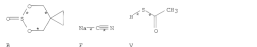
STAGE(2)
RGT V 507-09-5

PRO K 169954-91-0

RX(13): NCT K 169954-91-0
RGT M 1310-73-2 NaOH
PRO L 169954-92-3
SOL 108-88-3 PhMe, 7732-18-5 Water

RX(14): NCT L 169954-92-3, O 169954-93-2
RGT Q 109-72-8 BuLi
PRO P 169954-94-3
SOL 109-99-9 THF
NTE -5°, 0.5 h

RX(21) OF 28 COMPOSED OF RX(2), RX(6), RX(13), RX(14)
RX(21) B + F + V + O ==> P

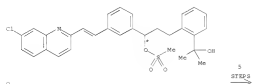
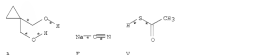


L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

STAGE(2)
RGT V 507-09-5
PRO K 169954-91-0
RX(13): NCT K 169954-91-0
RGT M 1310-73-2 NaOH
PRO L 169954-92-3
SOL 108-88-3 PhMe, 7732-18-5 Water

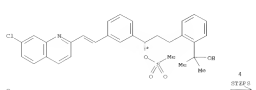
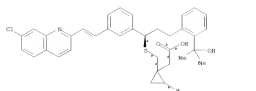
RX(14): NCT L 169954-92-3, O 169954-93-2
RGT Q 109-72-8 BuLi
PRO P 169954-94-3
SOL 109-99-9 THF
NTE -5°, 0.5 h

RX(23) OF 28 COMPOSED OF RX(1), RX(2), RX(6), RX(13), RX(14)
RX(23) A + F + V + O ==> P

F: CH 2
YIELD 79%

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L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

F: CH 2
YIELD 79%F: CH 2
YIELD 79%

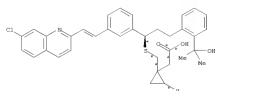
RX(12): NCT B 89729-09-9, F 143-33-9

RGT H 7681-82-5 NaI
PRO O 152922-71-9
SOL 108-88-3 PhMe, 68-12-2 DMF
NTE 70°

RX(16): NCT G 152922-71-9

STAGE(1)
RGT M 121-44-8 RL3N, T 124-63-0 MeSO2Cl

L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS on STN (Continued)

F: CH 2
YIELD 79%

RX(13): NCT A 39950-81-3
RGT C 7719-09-7 SOCl2, D 7087-68-5 Et3N(Pr-i)2
PRO B 89729-09-9
SOL 75-09-2 CH2Cl2
NTE 0-5°

RX(12): NCT B 89729-09-9, F 143-33-9
RGT H 7681-82-5 NaI
PRO O 152922-71-9
SOL 108-88-3 PhMe, 68-12-2 DMF
NTE 70°

RX(16): NCT G 152922-71-9

STAGE(1)
RGT M 121-44-8 RL3N, T 124-63-0 MeSO2Cl
SOL 68-12-2 DMF, 108-88-3 PhMe

STAGE(2)
RGT V 507-09-5

PRO K 169954-91-0

RX(13): NCT K 169954-91-0
RGT M 1310-73-2 NaOH
PRO L 169954-92-3
SOL 108-88-3 PhMe, 7732-18-5 Water

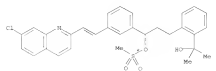
RX(14): NCT L 169954-92-3, O 169954-93-2
RGT Q 109-72-8 BuLi
PRO P 169954-94-3
SOL 109-99-9 THF
NTE -5°, 0.5 h

RX(24) OF 28 COMPOSED OF REACTION SEQUENCE RX(5), RX(14)
AND REACTION SEQUENCE RX(12), RX(6), RX(13), RX(14)
...S + T ==> O...
...B + F + V + O ==> P

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L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS ON STM (Continued)



O

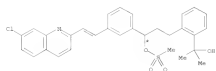
START NEXT REACTION SEQUENCE



B

F

V



O

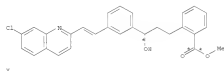
4
STEPSPr. CM 3
YIELD 79%

L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS ON STM (Continued)

SOL 109-99-9 T8F

RTE -0.5, 0.5 h

EX(18) OF 28 COMPOSED OF REACTION SEQUENCE EX(7), EX(5), EX(4)
AND REACTION SEQUENCE EX(1), EX(2), EX(6), EX(3), EX(4)
...X + 2 Y + 7 reagents O...
...X + F + V + O reagents



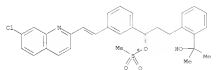
X



2 Y



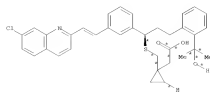
2

5
STEPS

O

START NEXT REACTION SEQUENCE

L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS ON STM (Continued)

Pr. CM 2
YIELD 79%

EX(7) RCT X 142569-69-5, Y 75-16-1
RGT Z 7790-86-5 C6C13
FXO S 142569-70-8
SOL 109-99-9 T8F, 108-88-3 F8Me

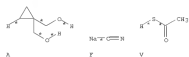
EX(5) RCT S 142569-70-8, T 124-63-0
RGT D 7087-68-5 E191Pr-112
FXO O 149954-93-2
SOL 108-88-3 F8Me, 75-05-8 MeCN

EX(2) RCT B 69729-09-9, F 143-33-9
RGT B 7681-82-5 NaI
FXO G 152322-71-9
SOL 108-88-3 F8Me, 68-12-2 DMF
RTE 704

EX(6) RCT Q 152322-71-9
STAGE(1)
RGT M 121-44-8 E13N, T 124-63-0 MeSO2Cl
SOL 68-12-2 DMF, 108-88-3 F8Me
RGT V 107-09-5
STAGE(2)

FXO K 169954-91-0
EX(3) RCT K 169954-91-0
RGT M 1310-73-2 NaOH
FXO L 169954-92-1
SOL 108-88-3 F8Me, 7732-18-5 Water
EX(4) RCT L 169954-92-1, O 169954-93-2
RGT Q 109-72-8 BuLi
FXO P 169954-94-3

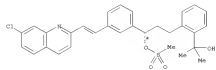
L3 ANSWER 16 OF 16 CASREACT COPYRIGHT 2009 ACS ON STM (Continued)



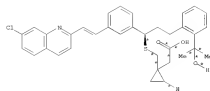
A

F

V



O

5
STEPSPr. CM 1
YIELD 79%Pr. CM 2
YIELD 79%

EX(7) RCT X 142569-69-5, Y 75-16-1
RGT Z 7790-86-5 C6C13
FXO S 142569-70-8
SOL 109-99-9 T8F, 108-88-3 F8Me

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L3 ARIZONA 18 OF 16 CALIBRANT COPPERIDET 2009 ACS on STM (Cont.Lined)
XX(15) NCT G 142569-70-8, T 124-63-0
      EGT D 7087-68-5 RHN(Pv-1)2
      PRO G 183945-93-2
      SOL 108-88-3 RHNMe, 75-05-8 MeCN
XX(11) NCT A 39590-81-3
      NCT C 7729-09-7 RNC12, D 7087-68-5 RHN(Pv-1)2
      PRO B 89729-09-9
      SOL 75-09-2 CR2C12
      HZE 0-5*
XX(12) NCT B 89729-09-9, F 143-33-9
      NCT H 7631-82-5 Na1
      PRO G 182920-71-9
      SOL 108-88-3 RHNMe, 68-12-2 DMF
      HZE 0*
XX(16) NCT G 182920-71-9
      STAGE(1)
      NCT W 121-64-8 RHN, T 124-63-0 Me802C1
      SOL 68-12-2 DMF, 108-88-3 RHNMe
      STAGE(2)
      NCT V 507-09-5
      PRO X 169954-91-0
XX(13) NCT F 169954-91-0
      NCT M 1310-73-2 NaOH
      PRO L 169954-92-1
      SOL 108-88-3 RHNMe, 7732-18-5 Water
XX(14) NCT L 169954-92-1, O 169954-93-2
      EGT Q 109-72-9 BuLi
      PRO P 169954-94-3
      SOL 109-99-9 THF
      HZE -5*, R, S h

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